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**Preliminary reliability evaluation of commercially available  
low-k interlayer dielectrics for space applications**

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## BRIEF SUMMARY

This paper reports the progress on a new NEPP initiative to assess the advances in the emerging low- $k$  dielectric materials in the state-of-the-art CMOS technology. The goal of this effort is to understand the materials properties, which have a potential impact on device performance and reliability in hostile space environments. This will facilitate the faster adoption of low- $k$  COTS products in NASA missions, thereby taking advantage of their enhanced performance.

The evaluation of electronic devices with low- $k$  dielectrics for possible use in space reliability will consist of the following program (accomplished tasks are marked with “✓”):

- ✓ Survey the currently available low- $k$  dielectric materials to determine the materials most likely to appear in electronic devices in the near future.
- ✓ Use percolation theory to determine the most likely porosity to be included in these materials.
- Extend percolation theory to predict thermal and mechanical properties of the most relevant porous materials.
- Evaluate the potential reliability performance of porous low- $k$  dielectric materials based on predicted thermal and mechanical properties.
- Measure experimentally the thermal and mechanical properties low- $k$  dielectric materials, both porous and non-porous.
- Evaluate actual COTS devices containing low- $k$  dielectrics.

**Part A** of this report covers the results of the initial phase of the study in which a summary is presented of the low- $k$  materials presently available for incorporation into device structures. **Part B** of the report presents the results of percolation theory, which was used to predict the most likely porosity structure in future devices. The steps to achieve understanding of the reliability criteria of low- $k$  dielectrics are discussed in section **Research Categorization**. The conclusions of this work are given in the **Extended Summary**.

## **PART A: LOW-K DIELECTRICS FOR CMOS DEVICES**

### **A.I. Introduction: Technology trends**

The advances in the electronic industry, which are driven by the necessity to produce integrated circuits (IC) with improved performance, are outlined in *The International Technology Roadmap for Semiconductors (ITRS 2001)* [1]. The conventional metals and dielectrics are unable to facilitate further progress, and new materials are sought to replace them. Less resistive metals (e.g., Cu) and low-dielectric-constant (low- $k$ ,  $k < 3.0$ ) materials, candidates for interlayer dielectrics (ILD) are needed to reduce the signal propagation delay. The low- $k$  materials will also suppress the cross-talk between interconnect wires. Although the *ITRS* shows the general path for improvements, a number of potential difficulties are identified. This has forced the companies to take different approaches, prioritizing differently the order of the changes along the way. Thus, at the 0.13  $\mu\text{m}$  node, some manufacturers will use organic spin-on dielectric (SOD), others will use silicate films (SOD or PECVD), whereas others will implement this change in next generation ICs. Plans for using low- $k$  dielectrics (at 0.13  $\mu\text{m}$ ) are in place at AMD, Motorola, IBM, Infineon, TSMC, and UMC, while Intel will adopt them later [2]. The main differences are dictated by the integration challenges of Cu and low- $k$ , which governs the ability to attain a low *effective* dielectric constant.

The fundamental limitations of all low- $k$  materials and the technical challenges from an integration point of view are given Ref. [2]. Further restrictions arise from the extendibility requirement. Preferably, the low- $k$  ( $k \sim 2.7$ ) material should facilitate the incorporation of porosity, which is the only road to achieving ultra-low- $k$  ( $k < 2.2$ ) values for the next-generation ILD. It is believed that this condition will rule out the CVD materials for the 0.10  $\mu\text{m}$  node. The embedded porosity will further compromise the mechanical and thermal properties of the material, as well as the compatibility with some IC production steps.

This deterioration of a spectrum of material characteristics raises serious concerns over using IC with low- $k$  and ultra-low- $k$  dielectrics in harsh space environments. However, little is known about the relevant properties and no reasonable performance assessment or comparison with Al/SiO<sub>2</sub> CMOS technology is feasible at this time. Conducting the necessary research is further complicated by the large number of ILD candidates with high commercialization potential, and by the proprietary nature of the materials fabrication. Nevertheless, extensive experimentation is imperative for the successful implementation of the new Cu/low- $k$  CMOS technology in future space missions. The immediate need for such research is dictated by the appearance of such devices on the market [3] and by the increasing importance of the commercial off-the-shelf (COTS) program for NASA. The successful low- $k$ /Cu integration allows for 30% increase in speed and performance, and thereby it carries direct benefits to space exploration. ASIC devices are now available to designers, and the >1.5 GHz G4 microprocessors built with this technology, are expected to appear on the market.

## A.II. Potential concerns for space applications of low- $k$ COTS

The porous low- $k$  dielectrics are *inhomogeneous* materials. As such, many of their physical properties *do not scale* as a superposition of air and low- $k$  solid with the appropriate proportions. Abrupt transitions can occur under such conditions, which are not encountered during production and normal device operation, but are seen in space environments. This may cause devices, which are reliable under normal operation, to fail when used in space. The full extent of such complications for low- $k$  COTS in NASA missions, is not known, and must be determined experimentally when the technology becomes available and mature. However, some anticipated scenarios can be addressed using raw materials or simple device or test structures; this will benefit their faster implementation in NASA missions. Such examples are given below.

### A.2.1. Thermal conductivity

Most of the low- $k$  candidates show thermal stability in the temperature range seen during production. MSSQ is stable in the 450-600 °C range [4], and SiLK can be processed below 450°C [5]. The thermal conductivity, however, decreases rapidly with the incorporation of porosity, as heat conduction is limited to the solid phase of a porous material. Some studies show a >10 times decrease for materials with ~20% porosity [6] ( $k \sim 2.1$  generation). Thus, a COTS device operating normally at <85 °C may not survive high-temperature environments, due to the inability to dissipate heat sufficiently fast. Furthermore, for porosity above the percolation threshold of the solid phase, the thermal conductivity diminishes. An excellent example for suppressed heat conductivity is the space shuttle heat shield, which is made of a porous low- $k$  candidate material – aerogel.

### A.2.2. Mechanical strength

The low- $k$  ILD candidates are mostly polymers, containing a large fraction of relatively weak bonds (C-H, O-H, etc.) and are susceptible to plastic deformation. They also contain “free volume” – open-volume areas depleted of bonds, which move under applied stress. Thus, polymers are inherently weaker than SiO<sub>2</sub>. Their elastic moduli decrease dramatically with porosity. It is still unclear whether the hardness of low- $k$  films changes abruptly around the critical porosity volume, as some experiments seem to indicate. Thus, excessive vibrations, such as these encountered during launch, present a serious challenge, and may cause device failure through internal fracturing.

### A.2.3. Brittleness

The problems related to brittleness are not obvious, but are arguably one of the most serious. The transition from ductile to brittle state of a solid dielectric is a problem, which the industry must resolve in order to produce a reliable device package. The porosity, however, plays a dominant role in determining the ductile-to-brittle phase transition as a function of temperature. Highly porous materials are generally more ductile at room temperature, and the ductile-to-brittle transition occurs at lower temperature. Thus, one can envision a scenario in which this transition is shifted to below –60 °C, which meets the military standards. However, exposed to a lower temperature the material may fracture, which will render the device unusable.

#### *A.2.4. Permeability*

This is arguably the best-known property of porous materials, which undergoes a first order phase transition at the critical percolation porosity fraction. Molecules, atoms and ions, placed anywhere within the volume are capable of reaching any other area through percolation pathways. This may have impact on space-relevant reliability issues, such as corrosion, operation in ion-rich environments (especially O-rich), and moisture absorption. Other reliability aspects relevant to device integrity, such as metal diffusion through porous media and the stability of barrier layers, are completely unknown in conditions, which deviate from those relevant to the normal use and device production. They too must be investigated prior to using low- $k$  COTS in space.

#### *A.2.5. Radiation cross-linking*

The cross-linking of a polymer low- $k$  film must be kept within some tolerable limits in order to keep the device integrity. Too little polymerization will degrade the hardness, whereas too much will make the material brittle. The effects of electron irradiation on polymers are known [7]. Electron irradiation was used to produce non-porous low- $k$  films [8], but large pores could not be retained. Only recent advances allowed the incorporation of sub-nanometer pores in MSSQ (LKD film made by JSR). Electron beam curing effects are important, as they influence the characteristics of logic devices [9]; therefore, the control over the electron dose is of imperative importance for the final structural properties of the low- $k$  material. With this in mind, the electron exposure is virtually eliminated after device production, whereas the electron radiation in space will continuously increase the low- $k$  brittleness. Furthermore, cross-linking usually releases water. At large amounts, water condensation and/or corrosion may occur.

#### *A.2.6. Ion radiation*

Another concern is related to the use of low- $k$  COTS in O-radiation environment. The majority of the low- $k$  candidates are highly susceptible to oxidation, which changes dramatically their dielectric constant, in some cases more than twice [10]. This can destroy the signal synchronization, thus rendering a processor inoperable. As cross-linking by radiation, oxidation is associated with the release of water, and thereby with condensation and corrosion. Heavy ion radiation affects the dielectric behavior of polymers as well (shown for [11] polyimide, another low- $k$  candidate).

#### *A.2.7. Combined effects*

Effects, which are caused by the simultaneous action of two or more factors, are most difficult to predict. However, some of them are foreseeable. For example, the increased brittleness through electron irradiation may be within tolerance limits for a device in controlled thermal environment, but may be detrimental in thermal cycling, or continuous extreme thermal exposure.

### A.III. Candidate low- $k$ materials

Two methods for low- $k$  deposition – chemical vapor deposition (CVD) and spin-on – dominate the choice for the 0.13  $\mu\text{m}$  node. CVD is the traditional oxide-deposition technique, which is used also in other production stages. The wealth of experience makes appealing the extension of its use at and below the 0.13  $\mu\text{m}$  node. Major drawbacks, however, are the difficulties in embedding porosity and the increasing production cost for small-feature devices. Conversely, the cost of ownership of the spin-on process remains nearly independent on the feature size, and its extendibility to 0.10  $\mu\text{m}$  and beyond by incorporating porosity has been demonstrated. It is expected that these advantages will render the spin-on technique dominant for the 0.10  $\mu\text{m}$  node. At 0.13  $\mu\text{m}$ , however, the industry will be split almost equally over the use of the two techniques.

#### A.3.1. CVD materials

The products of Applied Materials (*Black Diamond*) and Novellus (*CORAL*) are expected to dominate the next-generation CVD low- $k$  ILD's. Other noticeable CVD products are available from ASM (*Aurora*) and Dow Corning (*Z3MS*). The *Black Diamond* and *CORAL* films have the highest commercialization potential and they are expected to almost entirely dominate the CVD market.

- *Black Diamond* (Applied Materials):  $k = 3.0\text{-}2.1$

*Black Diamond* is a silicon-oxide based film ( $\text{SiCOH}$ ), which has been successfully integrated in a 8-layer Cu damascene process with BLOk (barrier low- $k$ ) diffusion barrier film. This scheme has shown 35% capacitance reduction relative to oxide/nitride. The *Black Diamond* is a moisture and fracture resistant film with sufficient hardness and good thermal conductivity.

- *CORAL* (Novellus):  $k = 3.3\text{-}2.4$

The *CORAL* family of low- $k$  films is another carbonaceous film ( $\text{SiCOH}$ ), structurally similar to the Applied Materials' *Black Diamond*, but with probably lower C and O content. The integration of the *CORAL* family films has also been demonstrated.

The dielectric constant in the  $\text{SiCOH}$ -type materials can be tuned by varying the C content. This affects the local structural composition, which results in embedded sub-nanometer porosity. This porosity tuning is limited, thus rendering the CVD method unsuitable for the production of  $k < 2.1$  ILD's. The CVD materials are hard and have good thermal conductivity, which governs their superior performance in the integration process compared to the spin-on materials.

#### A.3.2. Spin-on materials

Spin-on materials come in the form of organic and inorganic polymers or  $\text{SiO}_2$  type sol-gel materials (aerogels, xerogels). The sol-gels are films with bi-continuous solid and open phases. The percolated porosity creates complications in the material's integration and requires the use of capping layers. Sol-gel films have been available for the longest time; however, they are not favored by the industry. The present state-of-the-art sol-gels are available from Honeywell Electronics:

- *Nanoglass* series (Honeywell Electronics):  $k = 2.2$ -1.3 (highly tunable)  
*Nanoglass* has excellent adhesion strength and satisfactory mechanical properties, which degrade at higher porosity. *Nanoglass E* exhibits  $k = 2.2$  and contains  $\sim 2.0$  nm sized pores. *Nanoglass E* has been successfully integrated through the first and second metal levels of a copper dual damascene interconnect structure.

The most promising spin-on materials are hybrid (organo-inorganic), organic, or inorganic polymers. They are produced from a mixture of a low molecular weight polymer resin and a sacrificial polymer (porogen) [12]. Wafers are coated with a solution of the two components, and the solvent is driven out by a mild bake ( $<100$  °C). The copolymer is then thermally cured ( $200$ - $250$  °C) to force the phase separation of the two components and to vitrify the matrix polymer. During this stage, the porogen forms domains, whose size and density is governed by the curing conditions. The following high-temperature ( $\sim 450$  °C) bake out decomposes the porogen, which evacuates the film and leaves voids behind. Thus, the morphology of the porosity is strongly related to the porogen morphology during the low-temperature cure. Attention is directed to:

- *SiLK* (Dow Chemical):  $k = 2.65$ -1.6  
*SiLK* is a constantly evolving ILD, available in versions labeled by increasing letters (*I* version is presently available). This is the only material, which is currently available through *International SEMATECH*. IBM has selected *SiLK* for its 110 nm generation IC's, and their Cu-11 process integrates *SiLK* with Cu metallization.  
*SiLK* has a relatively low intrinsic  $k = 2.65$ . Due to its relatively good thermal and mechanical properties, it is a promising ILD candidate. Extendibility to smaller feature sizes has been demonstrated through incorporating porosity. However, the literature data show large pores, most recently quoting  $\sim 20$  nm size. This size is compatible with the pitch, and is therefore too large for implementation.
- *Dendriglass* (IBM):  $k = 2.8$ -1.6  
IBM has developed several technologies for templating pores in methyl-silsesquioxane (MSSQ:  $\text{CH}_3\text{SiO}_{3/2}$ ) films. Although IBM has no plans for commercializing these methods, it is highly probable that their production will be licensed to a third party. A wealth of research data is available in the literature. The pores are typically following closely a log-normal size distribution with  $\sim 2$  nm mean size, slightly dependent on the porosity fraction and the used porogens. The pore percolation threshold occurs at approximately 18-20% porosity. Porous MSSQ films have relatively good hardness and adhesion properties, however, films thicker than  $\sim 1$   $\mu\text{m}$  are brittle and they are prompt to fracturing. Low-temperature fracturing has also been observed in the past.
- *LKD* (JSR):  $k = 2.7$  and  $k = 2.2$   
JSR initially developed identical to the IBM-made MSSQ films. With time, their porosity templating methods evolved towards smaller pores, and presently JSR is working on incorporating sub-nanometer porosity. *LKD 2.7* may be possible to obtain through *International SEMATECH* providing non-disclosure terms are agreed.

- *FOx*, *XLK* (JSR):  $k = 2.8$  and  $k = 2.2$

The Dow Corning films are based on hydrogen-silsesquioxane (HSSQ:  $\text{HSiO}_{3/2}$ ), similar to MSSQ with methyl radicals ( $\text{CH}_3$ ) replaced by H. The *XLK* films are similar to the *FOx*, but contains ~20% nanotemplated porosity with similar pore size distribution to the MSSQ films. The major difference with MSSQ is that HSSQ films are highly hygroscopic and require a moisture barrier (usually SiC).

Other spin-on materials are available from Honeywell (*HOSP*, *GX-3*, *FLARE*), but are expected to have less impact on the market.

#### A.3.3. Alternative approaches

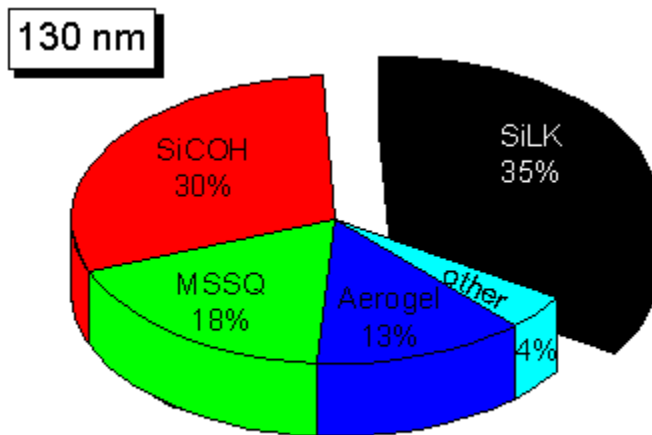
Most notable among the alternative approaches is the self-assembling monolayers (*SAM*). Such efforts are in place at Sandia and Pacific Northwest National Labs. The main attraction of these methods is in the arrangement and composition of porosity and the ability to manipulate the film properties. Usually, *SAM* films have superior physical properties to all other approaches; however, film growth is unacceptably slow. They will not be adopted by the industry in the near future (at least by 2010).

### A.IV. Evaluation of commercialization potential and selecting research targets

It is not trivial to predict the market share for the ILD materials for the 0.13 nm technology node; however, several important factors should be considered. First, CVD-grown materials have been used for many years and their integration does not create extraordinary challenges. Furthermore, recently developed methods for generating porosity on atomic level will extend their applicability far beyond the previously thought limits. Thus, despite the increasing cost of ownership, their track record may be decisive for their selection over the spin-on dielectrics. Another factor is the only successful integration of low- $k$  ILD (*SiLK*) and Cu in a production scheme. Having such products

available may have a significant impact on the market.

An expectation for the distribution of the ILD's is shown in the Figure 1. Note: this graph excludes  $\text{SiO}_2$  (Intel). The relative contributions were comprised after taking into consideration the opinions of different low- $k$  and device manufacturers regarding the low- $k$  properties and the difficulties in their integration. It should be kept in mind that solutions for many problems are still being pursued. The faith of these efforts can change the shape of this graph significantly.



**Figure 1.** Expected market share for different ILD candidates. Since it has already entered production, *SiLK* is considered under its trade name. *SiCOH* combines CVD CORAL and Black Diamond, and *MSSQ* combines all trade names with this material.



It is expected that approximately a third of the 0.13 nm products on the market will be made with *SiLK*. A potential increase of this fraction depends on the success of the IBM-Dow collaboration, which medium-size companies may follow. Potential problems may force these companies to choose the CVD (SiCOH) materials. Being an alternative to *SiLK*, MSSQ will also have a significant role on the market, and its impact also depends strongly in the *SiLK* implementation. Other materials, which require attention, are the aerogels and xerogels, most notable of which is *Nanoglass*.

The market distribution of the low- $k$  ILD's for the 0.13 nm technology node will determine that for the 0.10 nm generation ILD's. CVD-ILD's are likely to be abandoned unless methods are found to create highly porous films. Aerogels/xerogels may play larger role in future generations, for which porous ILD's will have percolated porosity regardless of the fabrication method.

The above considerations determine the materials with highest commercialization potential, and thereby with the largest impact on the NASA COTS program. Thus, the most suitable materials for future research are (in order of importance):

1. Spin-on: ***SiLK*** and **MSSQ** (*Dendriglass*, *LKD*, *XLK*)
2. CVD: **SiCOH** (*Black Diamond* and *CORAL*)

## **PART B: MODELING OF MATERIALS PROPERTIES**

### **B.I. Introduction: Percolation models**

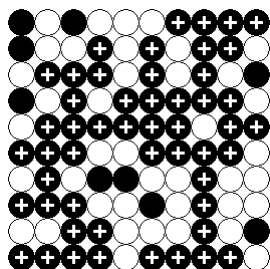
Computer-based models built on percolation theory [15-17] are especially suitable for studies of porous materials. They provide the basis for describing the transport properties of *inhomogeneous* media, which are characterized by morphology-dependent phase transitions, which *do not occur* in *homogeneous* materials. Such models have been successfully utilized in diverse areas, such as micro-fluidics, selective catalysis, molecular separation, chemical sensing, electro-optics, and microelectronics. In this work, simple models are utilized in a qualitative investigation of the relationship between the morphology of the porosity and the technology requirements given in the *ITRS* [1].

A square lattice site percolation is considered here as an example of a two-dimensional (2D) percolation model. A pore occupies a site in a  $L \times L$  square cell with a probability  $p$  ( $0 \leq p \leq 1$ ). If two adjacent sites are occupied, the respective pores are considered connected, e.g., allowing an imaginary particle to percolate from one pore to the other. All accessible pores to an imaginary particle placed in a given pore form a cluster. Clusters grow in size with the increase of porosity. At some critical value of  $p$ , denoted as percolation threshold,  $p_c$ , an infinite cluster is formed. In the finite-scale computer model, this is represented by the creation of a pathway through connected pores, spanning across the cell. This phenomenon, which is one of the main subjects studied by the percolation theory, represents a first order phase transition.

An analogous three-dimensional (3D) site percolation model on a simple cubic lattice ( $L \times L \times L$ ) is also considered here.  $L = 1000$  for the 2D and  $L = 100$  for the 3D cells were chosen as a compromise for obtaining a reasonable accuracy without using an excessive amount of computer time. Precise calculations of the respective percolation thresholds lie outside of the scope of this work. Their values are known with high accuracy:  $p_c(2D) = 0.592746$  and  $p_c(3D) = 0.311600$  [18]. The 2D and 3D models have many similar qualities. An important difference is the coexistence of two continuous phases (solid and open) for  $p_c < p < (1 - p_c)$  in the 3D case.

In both models, the clusters were separated into two groups: isolated clusters, which do not contain a percolation path to any of the surfaces, and open clusters, which extend to at least one side of the cell. The ratio of the sum mass (number of occupied sites) of all open clusters and the sum mass of all pores defines the open porosity fraction,  $F_{open}$ .  $F_{open}$  is a suitable parameter to demonstrate percolation effects, and a comparison with  $p_c$  is used here for model validation. For calibration purposes,  $F_{open}$  is calculated per side. Care is taken to avoid multiple counting of non-percolation open clusters, which reside on two or more surfaces. Although this expression does not affect  $p_c$ , the comparison with the analytical result that  $F_{open}$  approaches  $1/L$  for  $p \rightarrow 0$  provides a useful calibration. Calculated also is the density of the isolated clusters, defined as number of clusters per unit volume (cell volume:  $L^2$  in 2D;  $L^3$  in 3D). These results are nearly independent on the cell size for a sufficiently large cell. The density of single pores, multiple-pore clusters and all isolated clusters are monitored separately as a function of  $p$ .

The results are presented as a function of the *loading probability*,  $p$ , which is sometimes referred to as *number density* ( $n$ ). The *reduced number density*,  $\eta$ , is the more appropriate parameter when actual pore shapes are considered. The relationship between  $\eta$  and  $n$  is  $\eta = n \times f$ , where  $f$  is the *filling factor*, representing the available volume in which pores can be placed.



**Figure 1.** A representation of a 2D site percolation model on square lattice with disk-like shaped pores (black). Sites are filled randomly with  $p = 0.6$  ( $p_c \approx 0.593$ ) and the pores, which belong to the percolation cluster, are marked with a “+” sign.

As an example, consider discs with a diameter  $d = 1$  (the spacing between neighbor sites) in the 2D square model (Figure 1). When two neighbor sites are occupied (Figure 1, solid discs), the two discs touch in one point, through which a percolation path can pass. In such an arrangement, when all sites are occupied ( $p = 1$ ) a part of the cell area is inaccessible to the disks (no disk can be placed there). Therefore, the available volume fraction is  $f = \pi/4 \approx 0.7854$ , and percolation, using the values from Ref. [18], occurs at  $\eta_c = 0.465542$ . An analogical example for 3D considers spheres with  $d = 1$ , which gives  $f = \pi/6 \approx 0.5236$  and  $\eta_c = 0.163153$ .

The use of an adequate model for representing the subject is critical for obtaining valid quantitative results. However, it has been demonstrated that the reduced number density carries little model dependence for disks (2D) and spheres (3D) [19]. The present study sets the stage for future improved representations of the porous dielectrics perhaps utilizing the Bernal model for randomly packed hard spheres [20]. An even more realistic scenario is to enable the pores to coordinate on a distance larger than 1 (beyond the nearest neighbors) [21,22]. Inherent features to the low- $k$  production method may require a careful treatment of the interactions, which may shift the percolation threshold to either higher or lower values [23]. Other models, considering pores comprised of a hard core and a soft shell [24], may also be suitable.

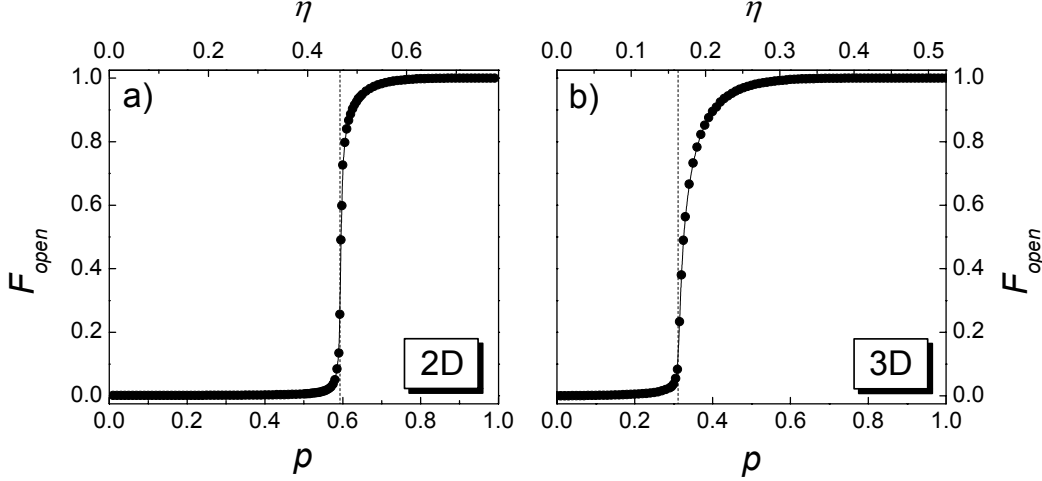
## B.II. Facilities

The program code used for these calculations was written in a Matlab environment, and the calculations were done on a 1 GHz personal computer with 512 Mb memory. Matlab is available at no cost to JPL employee through the Design Hub, for which a site license is issued. The code written for this purpose utilizes a number of functions specifically designed for Matlab for image analysis applications. Their utilization enables this preliminary research on reasonably large cells without the use of a supercomputer.

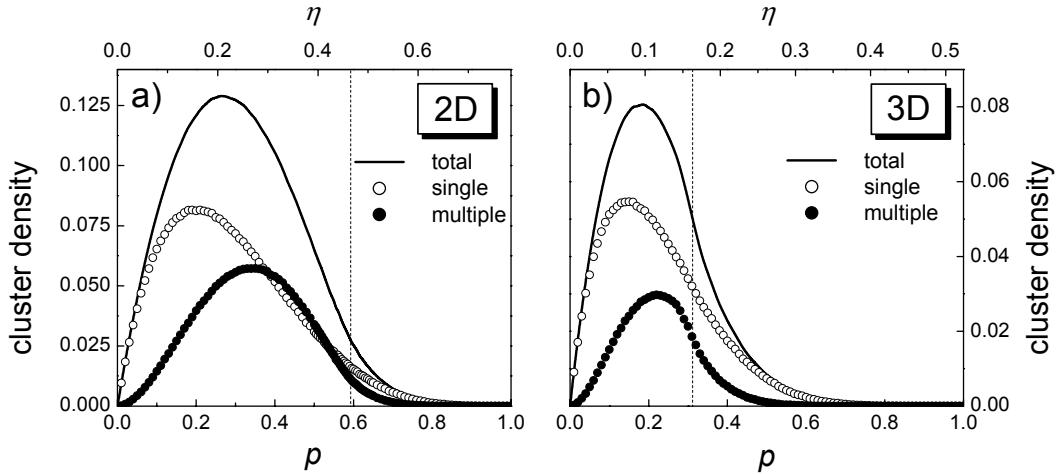
Future progress with more adequate models may require a more powerful computer. Two supercomputers, a CRAY SV1-1A and a SGI ORIGIN2000, are also available at no cost to JPL-users. They can be used with already developed routines for simulation of porous materials [e.g., 24].

### B.III. Preliminary results

Figure 2 shows the open porosity fraction,  $F_{open}$ , as a function of  $p$  for the 2D (Figure 2(a)) and 3D models (Figure 2(b)). The top scales show the reduced number density,  $\eta$ , using the filling factors for disks and spheres, respectively. The percolation thresholds for both cases, whose values are adopted from Ref. [18], are shown with vertical lines.



**Figure 2.** Open porosity fraction of site percolation models: **(a)** two-dimensional on a square lattice; **(b)** three-dimensional on a cubic lattice. The respective percolation thresholds  $p_c = 0.592746$  (2D) and  $p_c = 0.311600$  (3D) are shown with vertical lines. The top scales give the reduced number densities for disks and spheres, respectively.



**Figure 3.** Densities of isolated clusters in site percolation models: **(a)** two-dimensional on a square lattice; **(b)** three-dimensional on a cubic lattice. Shown are the total density (solid line), and the densities of single pores (open symbols), and multiple-pore clusters (solid symbols). As in Figure 2, the respective percolation thresholds are marked with vertical lines, and the top scale shows the respective reduced number densities for discs (2D) and spheres (3D).

The cluster density results from the 2D and 3D models are presented in Figure 3(a) and 3(b), respectively. The vertical lines mark the percolation thresholds in the two cases. Identical symbols are used to represent the corresponding data in both sub-plots: solid line for the total isolated cluster density, open circles for the density of single pores, and solid circles for the multiple-pore cluster density.

#### B.IV. Discussion

A meaningful dielectric constant of the considered solid must be assumed in order to relate the present results to porous low- $k$  dielectrics and investigate their properties against the guidelines given in the *ITRS* [1]. A realistic approach requires the assessment the existing low- $k$  materials with high commercialization potentials, such as SiLK ( $k = 2.65$ ) and MSSQ ( $k = 2.70$ – $2.85$ ). A number of other non-porous spin-on materials also exhibit dielectric constants in the 2.6–2.9 range. Therefore, the assumption of  $k_0 = 2.7$ – $2.8$  is in a reasonable range.

A simple superposition model can be considered to calculate the amount of required embedded porosity, with which a given preset  $k$ -value will be achieved. The porous dielectric can be represented by two slabs – one, consisting of the compressed solid material without the porosity with dielectric constant  $k_0$ , and a layer of air ( $k \approx 1$ ) with volume equal to that of the initial porosity (“projected” porosity). The film thickness remains unchanged. Being area-independent, the thickness ratio of the air-slab and the whole film is equal to the porosity volume fraction,  $x$ .

$$x = \frac{k_0 - k_{eff}}{(k_0 - 1) \cdot k_{eff}},$$

where  $k_{eff}$  is the effective dielectric constant of two capacitors, having  $k = k_0$  and  $k = 1$ , connected in series.

This approach is known to be successful in representing porous materials, and has been utilized to calculate foaming efficiencies of volatile polymers, which were used to produce porous MSSQ films [12] in a wide porosity range. Thus, one can calculate the porosity fractions in low- $k$  materials, necessary to reproduce the development trends underlined by the *ITRS*. Given in *Table I* are the values of the effective dielectric constant (due to low- $k$  and etch-stop layers) and the requirements for the bulk low- $k$  values.

**Table I.** Extracts from ITRS [2]: the effective and bulk dielectric constants in microprocessor (MPU) technology. Bold text: manufacturable solutions exist; bold-underlined text: manufacturable solutions not presently known.

Year of production	2001	2002	2003	2004	2005	2006	2007
<b>MPU: Interlevel metal insulator – effective dielectric constant (<math>k</math>)</b>	3.0-3.6	3.0-3.6	3.0-3.6	<b>2.6-3.1</b>	<b>2.6-3.1</b>	<b>2.6-3.1</b>	<b><u>2.3-2.7</u></b>
<b>MPU: Interlevel metal insulator – bulk dielectric constant (<math>k</math>)</b>	< 2.7	< 2.7	< 2.7	< <b>2.4</b>	< <b>2.4</b>	< <b>2.4</b>	< <b><u>2.1</u></b>

Thus, values of  $k = 2.4$  can be achieved (with  $k_0 = 2.7\text{--}2.8$ ) with 7–9% porosity, whereas  $k = 2.1$  requires 17–19% porosity. A close inspection of Figure 2(b) in this context indicates a drastic difference in the properties of these two examples – the porosity load in the latter material is above the percolation threshold. A porous material with porosity above the percolation threshold has many drawbacks. The significant changes in mechanical strength and hardness may compromise its integration and may degrade its compatibility with processes such as chemical-mechanical polishing. Metal diffusion is strongly enhanced in a porous media. Alterations of reactive ion etch steps may occur due to the increased accessible surface area. The damascene metallization process may result in Cu lines with irregular geometry. The formation probability of a “killer pore”, which when filled with Cu during metallization shorts neighboring wires, increases abruptly above the percolation threshold; any part of the percolation cluster may form a “killer pore”. Therefore, apart from the gradual porosity increase, sharp changes in other properties can give rise to major technologically important challenges in the transition from the  $k = 2.4$  to 2.1.

In contrast to  $k = 2.1$ , the porosity in the  $k = 2.4$  dielectric appears to be optimized in terms of pore connectivity. The ~9% porosity in the solid with  $k \sim 2.8$  is comprised mostly of isolated clusters, whose density is at its maximum. Moreover, the  $k \sim 2.7$  material needs ~7% porosity, at which the single pore density is maximized, and thus minimum surface roughness is obtained. This is preferable at identical other properties, since such morphology will benefit a number of production steps.

## RESEARCH CATEGORIZATION

The extend of the research effort, necessary for achieving the appropriate technology readiness level for NASA missions, must be put in perspective and must be compared to the acquired knowledge understanding of the behavior and reliability of the present Al/SiO<sub>2</sub> CMOS technology. Decades of ground- and space-based investigations and learned experience have contributed to the acquired wealth of information. During this time, the CMOS technology was evolving, but none of the implemented innovations compares to the presently ongoing revolutionary changes to new materials. Their properties hold the key to the successful utilization of state-of-the-art devices in space environments. With the ever-increasing use of COTS components in present and future missions, immediate research initiatives are need to enable the timely transition of these advanced technologies, in particular the low-*k* ILDs, into space exploration projects.

Three categories of research are equally important for the implementation of low-*k* COTS technology in NASA missions. They are defined as follows:

### ***1. Materials properties***

This purpose of this research category is to extend the existing investigation of materials properties, carried out by academic and industrial institutions, to conditions relevant to space exploration. The subject is to understand the materials behavior, to uncover the limitations to their use in space environments, and to seek methods to overcome these difficulties. These investigations can be carried out on bulk materials or thin films, and do not necessarily require device fabrication.

### ***2. Performance of simple devices***

The purpose is to study device performance in space-relevant environments by monitoring any the characteristics of simple devices or test structures built with low-*k* dielectrics. This overlaps significantly with the materials investigations, as device performance and materials properties are closely related. However, the goal of these studies is to assess potential reliability issues in actual devices. The performance should be limited by the materials characteristics, not by the device structure.

### ***3. COTS performance***

In this stage, device performance is evaluated on actual COTS, thus taking into account the specific architecture. In contrast to the above categories, this one depends on the COTS manufacturer and the maturity of the technology. This category is emphasized strongly by the NASA/NEPP program; however, it will not be sufficient to guarantee low-*k* COTS acceptability by itself. For that, knowledge of materials and device performance is essential.

Presently, evaluation of COTS performance is neither feasible (only IBM has offered low- $k$  COTS devices on the market), nor adequate (due to the immaturity of the technology). In contrast, the materials properties and device performance investigations can be carried out at the present. They are independent on device architecture, and the fabrication of low- $k$  products has become highly reproducible, thus making the results independent on the source of the low- $k$  material. Such investigations can provide the fundamental knowledge needed for the proper evaluation of actual COTS when they become available. This action can minimize any delay of the implementation of the low- $k$  technology in NASA missions.

Computer-aided simulations of porous media, based on percolation theory can be used to complement to experimental materials studies. The expertise for developing adequate percolation models presently exists. A timely extension of this task can benefit from the leveraging of a NFFP (NASA Faculty Fellowship Program) sponsored summer position, awarded to a leading expert in percolation theory. His expertise can be utilized to model mechanical and thermal properties of porous low- $k$  dielectrics, and to uncover reliability issues, associated with the porosity structure. The results from such investigations will be validated through a comparison with experimental data, while the modeling tools will be used (after validation) to study low- $k$  behavior in environments, which are difficult to reproduce in a laboratory.



## EXTENDED SUMMARY

Due to the extent of the research needed to enable the low- $k$  technology use in NASA missions, investigation of all low- $k$  candidates is unjustifiable. The purpose of this survey of candidate low- $k$  dielectrics was to evaluate their commercialization potential in order to focus future research efforts on the most promising materials. One product, **SiLK** (Dow Chemical Company), has already been used in 130 nm state-of-the-art ASICs (IBM), and is an obvious choice. Approximately a third of all 130 nm CMOS devices are expected to use *SiLK* as an interlayer dielectric. The other promising dielectrics are grouped as materials, not by their trade name. CVD-deposited silicate films (**SiCOH**) are the choice of low- $k$  for companies, which plan to postpone the change of deposition technology to spin-on dielectrics. Chip manufacturers own CVD tools, and the expertise acquired in their use plays important role in selecting CVD dielectrics. Thus, it is expected that CVD low- $k$  will be used in approximately a third of all 130 nm devices. The largest providers for CVD low- $k$  (combining to >90%) are Applied Materials (with *Black Diamond*) and Novellus (with *CORAL* films). The third material worth attention is **MSSQ**, chemically similar to SiCOH, but spin-on deposited. Being an alternative to *SiLK*, the success of the MSSQ depends on the integration difficulties of *SiLK*, and solving the extendibility (to 100 nm) problem with *SiLK* (not done to-date). As a spin-on, MSSQ is an alternative to the CVD materials, which are inadequate for the 100 nm technology node. Considering these two facts, MSSQ can rapidly emerge as the low- $k$  choice of many companies, replacing SiLK and CVD low- $k$ .

Apart from using SiO<sub>2</sub> (Intel), approximately 80-85% of the 130 nm low- $k$  CMOS devices will be made with the above materials. They represent a suitable choice for future NASA / JPL research, which can be further limited by excluding the CVD low- $k$ . Despite their importance for the commercial market, the CVD materials will be used by one generation of COTS, which can be disregarded for space use. It is anticipated that the acquisition of data and knowledge needed for qualifying the technology will take longer than the life of this generation itself (~1.5-2 years), thus making the research unjustifiable. Conversely, the embedding porosity in spin-on dielectrics makes them usable in many COTS generations.

The properties of the low- $k$  dielectrics are significantly different from these of SiO<sub>2</sub>, and the behavior of low- $k$  COTS in hostile space environments can be very different. Due to the present unavailability of low- $k$  COTS devices, qualification of such parts is impossible. However, much relevant information can be learned from blanket films or using simple devices. Materials properties govern device behavior in a number of cases, and their understanding is imperative for the successful use of low- $k$  COTS in space, and for the timely transfer of this new technology to space exploration missions.

This work also explored the feasibility of utilizing computer simulations for understanding the properties of porous materials, such as the low- $k$  dielectrics. Simple percolation models were used successfully to compare the technology requirements for the bulk dielectric constant against the available materials. The necessary porosity load was related to the critical percolation, which determines transport properties in inhomogeneous media. It was found that these effects will take place at the  $k \sim 2.1$  generation ILD. The implications of these findings are that the present manufacturing

schemes will be inadequate for the production of  $k < 2.1$  ILD generations, and therefore reliability studies of such COTS parts will require different techniques, which will associate with different reliability issues.

This percolation approach to studying materials properties and their impact on device reliability provides an alternative and complementary means of understanding the low- $k$  dielectrics. The next logical step is to create an accurate representation of the morphology of the porosity in SiLK and MSSQ in order to study their thermo-mechanical properties. This will provide the alphabet one needs to read the results from future experiments. Thus, many of the discussed materials properties can be predicted, and the related reliability issues can be addressed before low- $k$  COTS devices are available on the market. Furthermore, these calculations can direct research funds into areas, where efforts are worth pursuing, and can prevent a waste of time and efforts in areas, where solutions do not exist.

The extension of the modeling effort will provide an excellent leverage for collaboration with the industry. Due to the proprietary nature of the low- $k$  materials, porous low- $k$  materials can only be obtained through such cooperation, which is thus invaluable for providing a timely transfer of information from the industry to NASA.

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